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Linearly-polarized optical transitions at type-II interfaces in the tight-binding approach

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Abstract. The sp^3 tight-binding method has been applied to calculate the in-plane anisotropy of optical matrix elements for indirect electron-hole radiative recombination at a type-II interface. It has been shown that, in type-II heterostructures with large band off-sets, the linear polarization of the photoluminescence vary in a wide range, including values ~100%, as a function of the tight-binding parameters characterizing the interface cations and anions. The behaviour of electron and hole quantum-confined states near the interface and their overlap has been analyzed as well.

Recently it has been demonstrated that, in type II zinc-blende-lattice multi-layered heterostructures grown along the [001] principal axis, the interfaces can induce a remarkable in-plane anisotropy. The anisotropy arises due to tetrahedral orientation of chemical bonds lying in the (110) and $(1\bar{1}0)$ planes. As a result the vertical photoluminescence (PL) is linearly polarized with the polarization reaching high values up to 80% in BeTe/ZnSe [1] and 21% in CdS/ZnSe [2].

In type II CA/C′A′ systems with large conduction- and valence-band offsets (~2 eV and ~1 eV for the BeTe/ZnSe pair) the penetration depth for an electron into the CA layer and for a hole into the C′A′ layer has the order of the lattice constant. Therefore in such a system the wavefunctions of an electron and a hole participating in the spatially indirect radiative recombination overlap remarkably only over few atomic planes. In this case the validity for the conventional envelope function approximation is questionable and one must instead use pseudopotential or tight-binding models.

We have applied the empiric tight-binding model sp^3 in the nearest-neighbor approximation, see [3], in order to find electron states quantum-confined within a C′A′ layer and hole states confined in a CA layer. For a (001)-grown structure, the carrier wave function in the state with the zero in-plane wave vector may be written as

$$\psi = \sum_{n,\alpha} C_n^{\alpha} \phi_{n\alpha}(x, y, z - z_n) \ , \tag{1}$$

where z is the growth direction [001], $z_n = na_0/4$, a_0 is the lattice constant, the integer n enumerates anion (for even $n = 2l$) and cation (for odd $n = 2l - 1$) atomic planes, $\phi_{n\alpha}$ are the planar atomic orbitals, and we take into consideration the orbitals $\alpha = s, p_{x'}, p_{y'}, p_z$. Hereafter we use the coordinate system with $x \parallel [100]$, $y \parallel [010]$ and $x' \parallel [1\bar{1}0]$, $y' \parallel [110]$.

For the C′A′ material we used the tight-binding parameters close to those presented for ZnSe by Vogl et al. [3]. The parameters for another material, CA, and for the interface atoms are indicated in caption to Fig. 1. Most of them coincide with those of C′A′ and only a few are different, in order to get the band gap $E_g(CA) = 4.3$ eV and the band off-sets

$$E_c(CA) - E_c(C'A') = 2.5 \text{ eV} \quad \text{and} \quad E_v(CA) - E_v(C'A') = 0.9 \text{ eV},$$

respectively for the conduction and valence bands.

The optical matrix elements for the emission of photons polarized along $x' \parallel [1\bar{1}0]$ and $y' \parallel [110]$ axes are calculated in the framework of the theory briefly outlined in [ ] and given by

$$M_\alpha = i\frac{a_0 m_0}{4\hbar} \sum_{l=0,\pm 1\ldots} V_l^\alpha ,$$

$$\begin{aligned} V_l^{x'} &= V_{sa,pc} C_{2l}^s C_{2l-1}^{x'} + V_{pa,sc} C_{2l-1}^s C_{2l}^{x'} , \\ V_l^{y'} &= V_{sa,pc} C_{2l}^s C_{2l+1}^{y'} + V_{pa,sc} C_{2l+1}^s C_{2l}^{y'} . \end{aligned} \tag{2}$$

Here M_α is the interband matrix element of the momentum operator $\hat{p}_\alpha$ for $\alpha = x'$ and y', $V_l^{x'}$ is the contribution to $M_{x'}$ from interatomic transitions between the anion plane $2l$ and cation plane $2l-1$, $V_l^{y'}$ is that for the pair of planes $2l$ and $2l+1$, $V_{sa,pc}$ and $V_{pa,sc}$ are the anion-cation transfer tight-binding parameters, C_n^s is the s-orbital coefficient in the expansion (1) for the lowest quantum-confined electron state in the conduction band, C_n^α is the similar p_α-orbital coefficient for the lowest quantum-confined heavy-hole state in the valence band. We exploit the theory by Lew Yan Voon and Ram-Mohan [ ] where the intrasite contribution to the optical matrix elements is ignored and the interatomic transitions between the planes $2l$, $2l-1$ and $2l$, $2l+1$ are coupled with photons polarized respectively along $[1\bar{1}0]$ and $[110]$.

Fig. 1 illustrates the calculation of the polarization degree, P_{lin}, defined as the ratio $(I_{1\bar{1}0} - I_{110})/(I_{1\bar{1}0} + I_{110})$, where I_{110}, $I_{1\bar{1}0}$ are the intensities of the PL components polarized along the corresponding axes. In the figure we present results for the interface

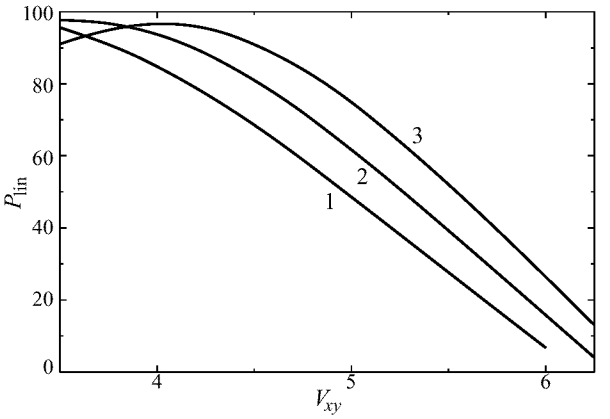

Fig. 1. The degree of PL in-plane linear polarization calculated as a function of the tight-binding transfer parameter V_{xy} for the C′A chemical bond at the (001) interface between the binar compositional materials CA and C′A′. The other parameters used are as follows: the diagonal energies $E_{sa} = -11.2$ eV, $E_{sc} = 2.8$ eV, $E_{pa} = 2.0$ eV, $E_{pc} = 8.8$ eV in CA and $E'_{sa} = -11.8$ eV, $E'_{sc} = 0.02$ eV, $E'_{pa} = 1.5$ eV, $E'_{pc} = 6.0$ eV in $C'A'$; the interatomic transfer matrix elements $V_{ss} = -6.2$ eV , $V_{xx} = 3$ eV, $V_{sa,pc} = 3.5$ eV and $V_{pa,sc} = 6.3$ eV are chosen to be the same in CA, C′A′ and at the interface bonds, $V_{xy} = 6$ eV in CA, C′A′ and arbitrary at the interface. As for the diagonal energies $\tilde{E}_{sa}$, $\tilde{E}_{sc}$ and $\tilde{E}_{pa}$ at the interface atoms C′ and A, the average values $(E_{sa} + E'_{sa})/2$ etc. are taken. Curves 1, 2 and 3 are obtained respectively for $\tilde{E}_{pc} = 6.4$ eV, 7.4 eV and 8.4 eV.

C′A assuming the interfacial bonds to lie in the (110) plane containing the $[1\bar{1}0]$ and [001] axes. For the CA′ interface the results are similar but in this case the polarization is directed along [110]. Thus, the polarization follows the direction of the interface chemical bonds as predicted in [ ]. Note that the parameter V_{xy} for the interface cations and anions can remarkably differ from its value in the bulk semiconductor C′A and is considered as an indipendent variable. We see that, provided all other parameters are fixed, values of P_{lin} increase with decreasing V_{xy} from 6 eV to 4 eV and exceed 80% for $V_{xy} < 4.2$. The polarization is almost insensitive to the electron and hole confinement energies within a wide energy range. However we remind that here we consider only the electron and hole states with $k_x = k_y = 0$.

To demonstrate the behaviour of the electron and hole wave functions near the interface, we presented in Table 1 values of C_n^α for n between -4 and 4 assuming the C′ and A interface planes correspond to $n = -1$ and $n = 0$ respectively. One can see that the conduction-band coefficients C_{2l}^s at anions or C_{2l-1}^s at cations rapidly decrease with increasing l whereas the valence-band coefficients decay the C′A′ material.

For completeness we presented in Fig. 2 the dependence $V^{x'}$ and $V^{y'}$ upon l. As predicted in [ ] the maximum contribution to $M_{x'}$ is given by the pair of the interface planes A′ and C and the main contribution to M_α comes from V_l^α with $|l| \leq 3$. The maximum contributions to $M_{x'}$ and $M_{y'}$ come from the planes $-1, 0$ and $0, +1$. According to Eq. (2), the ratio of these particular contributions is mainly given by

$$\eta = \frac{C_{-1}^s C_0^{x'}}{C_1^s C_0^{y'}} .$$

From Table 1 calculated for $V_{xy}(C'A) = 5$ eV, $E_{pc} = 7.4$ eV we have $\eta = 2.2$ and $(\eta^2 - 1)/(\eta^2 + 1) = 0.65$ which is close to $M_{x'}/M_{y'} = 2.06$ resulting in $P_{lin} = 62\%$.

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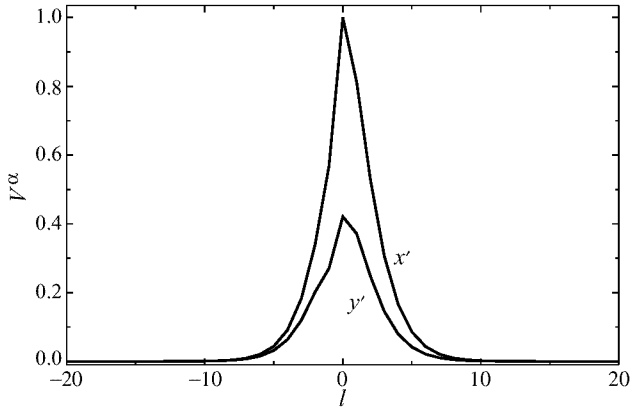

Fig. 2. Contribution of particular pairs of planes, $(2l, 2l - 1)$ and $(2l, 2l + 1)$, to the optical matrix elements, respectively in the x' and y' polarization.

Table 1. The unnormalized coefficients of the expansion (1) near the interface for the set of tight-binding parameters presented in caption to Fig. 1 and for $V_{xy}(C'A) = 5$ eV, $\tilde{E}_{pc} = 7.4$ eV.

Atom	A'	C'	A'	C'	A	C	A	C	A
n	−4	−3	−2	−1	0	1	2	3	4
C^s	−0.26	0.50	−0.17	0.27	−0.08	0.13	−0.04	0.06	−0.02
$C^{x'}$	0.05	−0.08	0.11	−0.2	0.36	−0.31	0.66	−0.41	0.95
$C^{y'}$	0.04	−0.01	0.10	−0.02	0.34	−0.07	0.64	−0.19	0.93

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